Quasiparticle spectrum of grain boundaries in d-wave superconductors

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Abstract

A grain boundary which separates domains with different orientation along the c-axis is analyzed. The coupling of two parallel superconducting planes whose order parameters are rotated leads to interesting properties which are expected to be common to other kinds of grain boundary. The density of states is enhanced at low energies. The number of localized states depends on the degree of misfit across the boundary. A continuum of zero energy states appears at certain values of the angle of rotation.

High temperature superconductors have been deeply studied since their discovery in 1986 [1]. These new materials are based on planar copper oxide structures that are insulating and present a phase transition to a superconducting state when they are doped. The microscopic models proposed [2] to explain the appearance of superconductivity in these materials point to a non conventional symmetry of the order parameter. Now, it seems that finally the d-wave model is fully accepted [3–14] as the correct one, at least for hole-doped superconductors. The determination of the pairing symmetry has been possible thanks to the experiments done using different techniques. Those experiments done in samples with grain boundaries have been especially important. It is well known that lattice distortions, such as grain boundaries, provide an intrinsic source of frustration in anisotropic superconductors because the order parameter follows the orientation of the lattice axes. These systems have been widely studied in the literature both experimentally [9–12,15–17] and [18–26]. First experimental results were controversial. Experiments reported by Sun and collaborators [15] showed the observation of a small but finite Josephson coupling between a conventional s-wave superconductor and a heavily twinned film of YBCO. This was interpreted as an evidence against d-wave symmetry. Josephson coupling across interfaces between two YBCO regions with crystalline axis misoriented by 45^o led Chaudhari and Lin [17] to the same conclusion. On the other hand, the detection of a half quantum of flux on tricrystal ring experiment [9,10] gave a clear evidence of the existence of nodes and lobes in the gap, supporting the d-wave model. Recently it has been reported an experiment [11] which, based on symmetry considerations, demostrate a pure d-wave order parameter in the tetragonal superconductor Tl2201.

However, the orthorhombic structure of YBCO allows for the existence of $d + s$ pairing symmetry. Direct evidence of this behavior has been found on the magnetic interference pattern of a sample with a single twin boundary [12], at which the direction of a and b axes reverse. As the junction is formed in the superconducting plane the whole system lacks periodicity. This fact introduces complexity in the study of the excitation spectrum. Latter has been studied [23] within the framework of the Bogoliubov-de Gennes (BdG) equations

and from ad hoc microscopic models. The excitation spectrum presents a zero-energy peak in the local density of states near the twinning plane. Here we show that a finite density of states at $E = 0$ can also be obtained in another kind of grain boundaries.

In the present article, a new type of grain boundary is analyzed, see Fig. 1. We consider two parallel superconducting planes with d-wave pairing symmetry. One of the planes has its order parameter rotated with respect to the other by an angle ϕ_0. Both planes are coupled by a hopping term t, which allows the exchange of electrons between the two planes. Interplane tunneling of Cooper pairs [27] could also be included in the model system but, for the sake of simplicity, we have not taken it into account. Notice an important difference between our system, where the grain boundary is formed between two planes, and grain boundaries usually considered in the literature with only one plane involved. Due to the symmetry of our system, the spin and momentum are conserved in the hopping process, contrary to what happens in other kind of grain boundaries, where translational invariance is violated. This fact opens us the possibility to obtain the whole spectrum and to study the characteristic features of grain boundaries avoiding quasiclassical approximations [28]. Despite of its simplicity, we expect the spectrum of our system to reproduce the same behavior than in plane grain boundaries. Besides, this kind of structure could not only be found in YBCO but also in other compounds. In particular, the case $\phi_o = \frac{\pi}{2}$ is equivalent to π-junctions [20,22,24]. It has also been suggested the possibility that this type of structures is formed in granular materials as well as during the growth process of the superconducting planes. A more realistic model should consider the coupling of two semiinfinite media but we expect that the main properties are captured by the present model.

We start from the mean field Hamiltonian

$$
\begin{aligned}
H = &\sum_{k\sigma} \xi_k c^\dagger_{k\sigma\alpha} c_{k\sigma\alpha} + \sum_{k\sigma} \xi_k c^\dagger_{k\sigma\beta} c_{k\sigma\beta} \\
&+ \sum_k \Delta_{k\alpha} c^\dagger_{k\sigma\alpha} c^\dagger_{-k-\sigma\alpha} + \sum_k \Delta^*_{k\alpha} c_{-k-\sigma\alpha} c_{k\sigma\alpha} \\
&+ \sum_k \Delta_{k\beta} c^\dagger_{k\sigma\beta} c^\dagger_{-k-\sigma\beta} + \sum_k \Delta^*_{k\beta} c_{-k-\sigma\beta} c_{k\sigma\beta}
\end{aligned}
$$

$$+\sum_{k\sigma} t c^{\dagger}_{k\sigma\alpha} c_{k\sigma\beta} + \sum_{k\sigma} t c^{\dagger}_{k\sigma\beta} c_{k\sigma\alpha} \tag{1}$$

where greek indices label the planes, $c^{\dagger}_{k\sigma\alpha}$ creates an electron with momentum k and spin σ in the plane α, and $\xi_k = \frac{\hbar^2 k^2}{2m} - \mu$ with μ being the chemical potential. This dispersion relation has been chosen because of its simplicity but the generalization to one with a different dependence on k is straightforward. The angle of rotation ϕ_o comes into the problem through the relative values of the order parameters:

$$\begin{aligned}\Delta_{\vec{k}\alpha} &= \Delta \cos 2\phi \\ \Delta_{\vec{k}\beta} &= \Delta \cos 2(\phi + \phi_o)\end{aligned} \tag{2}$$

To calculate the eigenvalues of this Hamiltonian the BdG equations are solved. After a straightforward calculation we obtain:

$$\begin{aligned}E_k^2 = \xi_k^2 + t^2 + \frac{\Delta^2}{2}[\cos^2 2\phi + \cos^2 2(\phi + \phi_0)] \\ \pm \{\frac{\Delta^4}{4}[\cos^2 2\phi - \cos^2 2(\phi + \phi_0)]^2 + 4\xi_k^2 t^2 \\ + t^2 \Delta^2 [\cos 2\phi - \cos 2(\phi + \phi_0)]^2\}^{\frac{1}{2}}\end{aligned} \tag{3}$$

This spectrum presents states at the Fermi level. These zero energy states, or nodes, are given by the equation:

$$\begin{aligned}\xi_k^2 = t^2 - \frac{\Delta^2}{2}[\cos^2 2\phi + \cos^2 2(\phi + \phi_0)] \\ \pm \Delta \mid \cos 2\phi + \cos 2(\phi + \phi_0) \mid \\ \times \sqrt{\frac{\Delta^2}{4}[\cos 2\phi - \cos 2(\phi + \phi_0)]^2 - t^2}\end{aligned} \tag{4}$$

From this equation it is clear that nodes can only exist if one of the following conditions is satisfied:

$$\mid \cos 2\phi - \cos 2(\phi + \phi_0) \mid \geq \mid \frac{2t}{\Delta} \mid \tag{5}$$

or

$$\cos 2\phi + \cos 2(\phi + \phi_0) = 0 \tag{6}$$

Two parameters are relevant: the hopping t between the planes and the angle ϕ_o. For small values of t the most relevant condition is (5) except for $\phi_0 = \pi/2$. On the other hand, for sufficiently large values of t, (5) is never fulfilled and the nodes are given by

$$\xi_k^2 = t^2 - \Delta^2 \cos^2 2\phi \tag{7}$$

with ϕ given by (6). The solution of eq.(4) in the first Brillouin zone is plotted in Figs. $2a$ and $2b$ for $\phi_0 = \pi/6$ where the influence of the hopping can be seen. The nodes appear in pairs. As the hopping increases, the distance between the nodes in a pair decreases. When (5) cannot be satisfied the nodes are aligned. The situation is different for $\phi_0 = \pi/2$ where a continuous line of nodes is obtained. It can be seen that as the hopping increases more values of ϕ satisfy (7) and when $t \geq \Delta$ there are nodes for any ϕ. This behavior is shown in Figs. $2c$ and $2d$. The continuous line of nodes implies the existence of a finite density of states at $E = 0$. This is only observed for values of ϕ_0 very close to $\pi/2$. In a superconductor with tetragonal symmetry values of $\phi_o > \pi/4$ correspond to non-equilibrium situations. However, they can appear if a current is applied, as well as in orthorhombic superconductors with non-equivalent axes, where similar features are expected.

The density of states shows a characteristic multi-peak structure due to van Hove singularities, which are associated to saddle points of E_k given by eq (3). It is worthy to note that we have started from a ξ_k which presents no saddle points. As can be seen in Fig. 3, the width of the peaks increases with the hopping reflecting the splitting of the Fermi surface. For high energies the density of states is a constant as in normal metals in 2D.

In general there are localized states at the grain boundary. Notice that we use localized states in the sense that for a given momentum there exist excitations with an energy E_k lower than the corresponding excitation energy in absence of grain boundary ($\phi_o = 0$).

$$E_{k\gamma} = \sqrt{(\xi_k \pm t)^2 + \mid \Delta_{\vec{k}\gamma} \mid^2} \tag{8}$$

where γ labels the index of the plane. The region of the Brillouin zone which presents localized states is displayed in Fig. 4. These states are mainly found inside the splitted Fermi

surface ($\xi_k = \pm t$) for the unfrustrated case and close to the values of ϕ which correspond to the nodes. The area of this region increases with t and ϕ_o. This kind of grain boundary in a 3D sample could be described as two coupled semiinfinite media. The localized states could not propagate into the bulk, but they would only exist at the boundary. The effect of the semiinfinite media can be introduced in terms of a self-energy. As a consequence, the extended states will have a finite mean lifetime. Note that, in a real sample, the planes are coupled in groups. In some cases it is only necessary to consider the coupling inside the groups. Thus, our results could be directly applied to double-layered systems.

In conclusion, we have studied a new type of grain boundary, which can appear in granular superconductors and, in general, during the growth process. The excitation spectrum displays new interesting features which seem to be common to other grain boundaries. Our model system can be found in any superconductor with d-wave symmetry and not only in the ones with orthorhombic structures as the widely studied twin boundaries [12,15,21–24] in YBCO. The simplicity of our model allows us to explore the whole spectrum. In more complex systems where not only two planes but two semiinfinite media are coupled, the spectrum is expected to display similar properties at the boundary. The quasiparticle spectrum has nodes such that the positions of the latter depend on the coupling constant between the planes and on the relative angle of the order parameters. The multi-peak structure of the density of states reflects the saddle points of the quasiparticle spectrum, while the enhancement at low energies is due to the existence of localized states.

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FIGURES

FIG. 1. Sketch of our model system

FIG. 2. The nodes of the spectrum for $\phi_0 = \frac{\pi}{6}$, $t = 0.4\Delta$ in Fig. 2a and $t = 0.8\Delta$ in Fig. 2b, and for $\phi_0 = \frac{\pi}{2}$, $t = 0.8\Delta$ in Fig. 2c and $t = 1.2\Delta$ in Fig. 2d, are plotted. $\phi_0 = \frac{\pi}{2}$ displays an unusual behavior with a continuum line of nodes in contrast to eight nodes found in almost all the other cases. The influence of the hopping can also be seen. For $\phi_0 = \frac{\pi}{6}$ the nodes in a pair tend to be closer as the hopping increases (see text). For $\phi_0 = \frac{\pi}{2}$ as the hopping grows an increasing number of nodes is obtained. Here, k is given in units of a^{-1}, where a is the lattice constant. Finally, $\frac{\hbar^2\pi^2}{2ma^2} = 40\Delta$ and $\mu = 10\Delta$.

FIG. 3. The density of states for $\phi_0 = \frac{\pi}{6}$, $t = 0.8\Delta$ and $t = 2\Delta$ is plotted. The enhancement of the density of states at low energies increases with the hopping. The hopping also influences the width and number of peaks which appear.

FIG. 4. The figure shows the region of the Brillouin zone (BZ) which displays localized states for the case $\phi_0 = \frac{\pi}{6}$ and $t = 0.8\Delta$. Units of k and values at the boundaries of BZ are the same as those given in the caption of Fig. 2

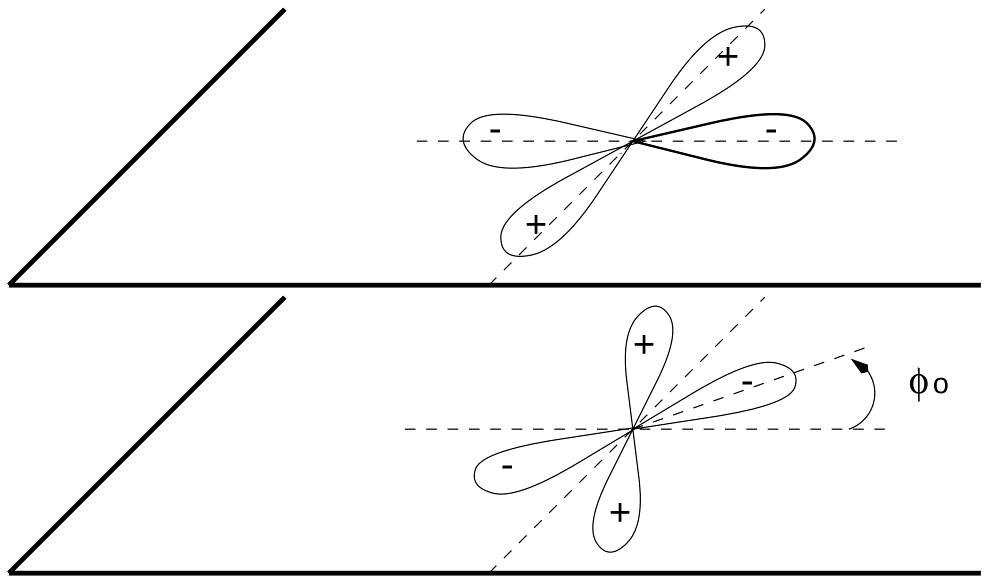

Fig. 1

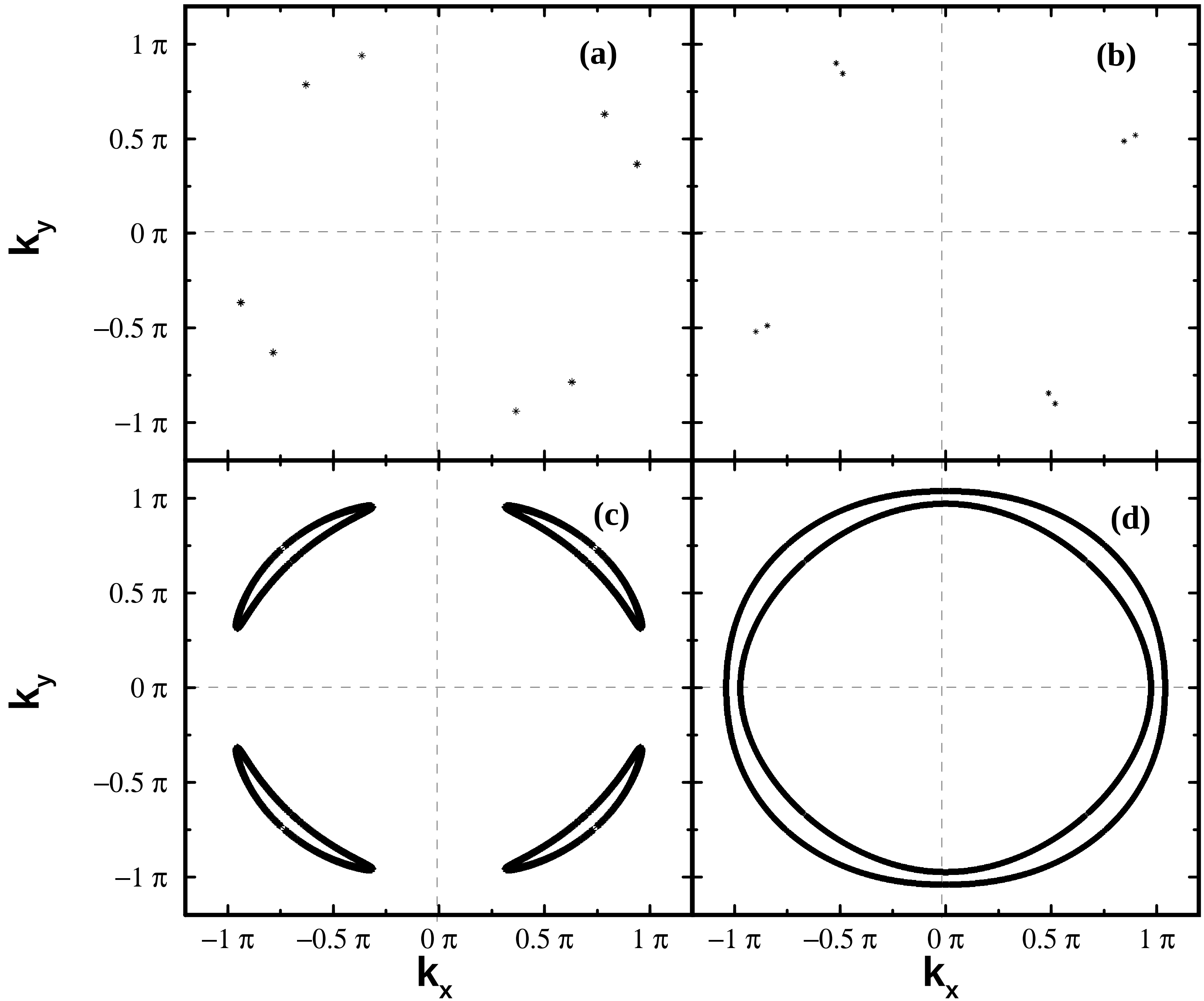

Fig. 2

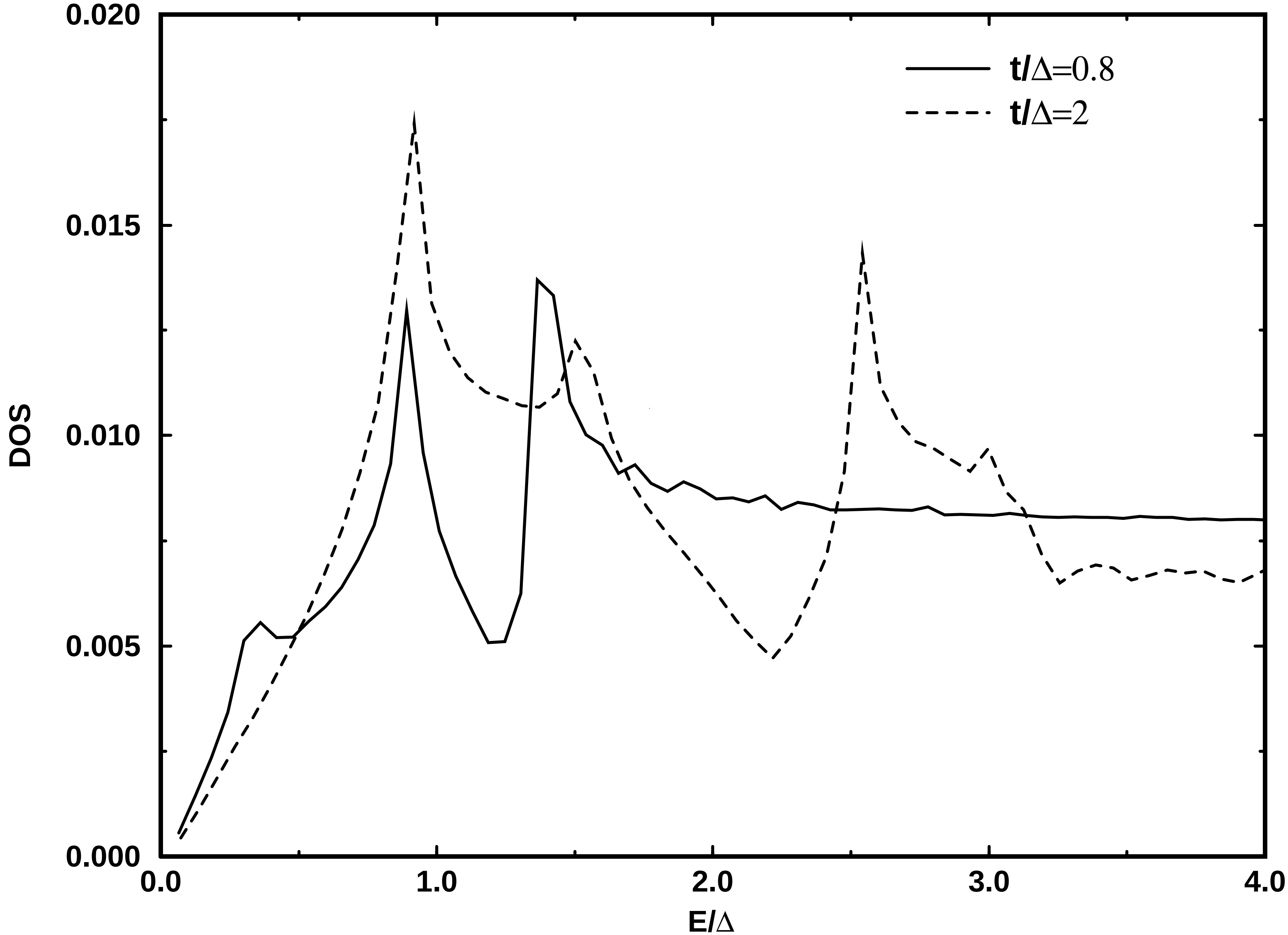

Fig. 3

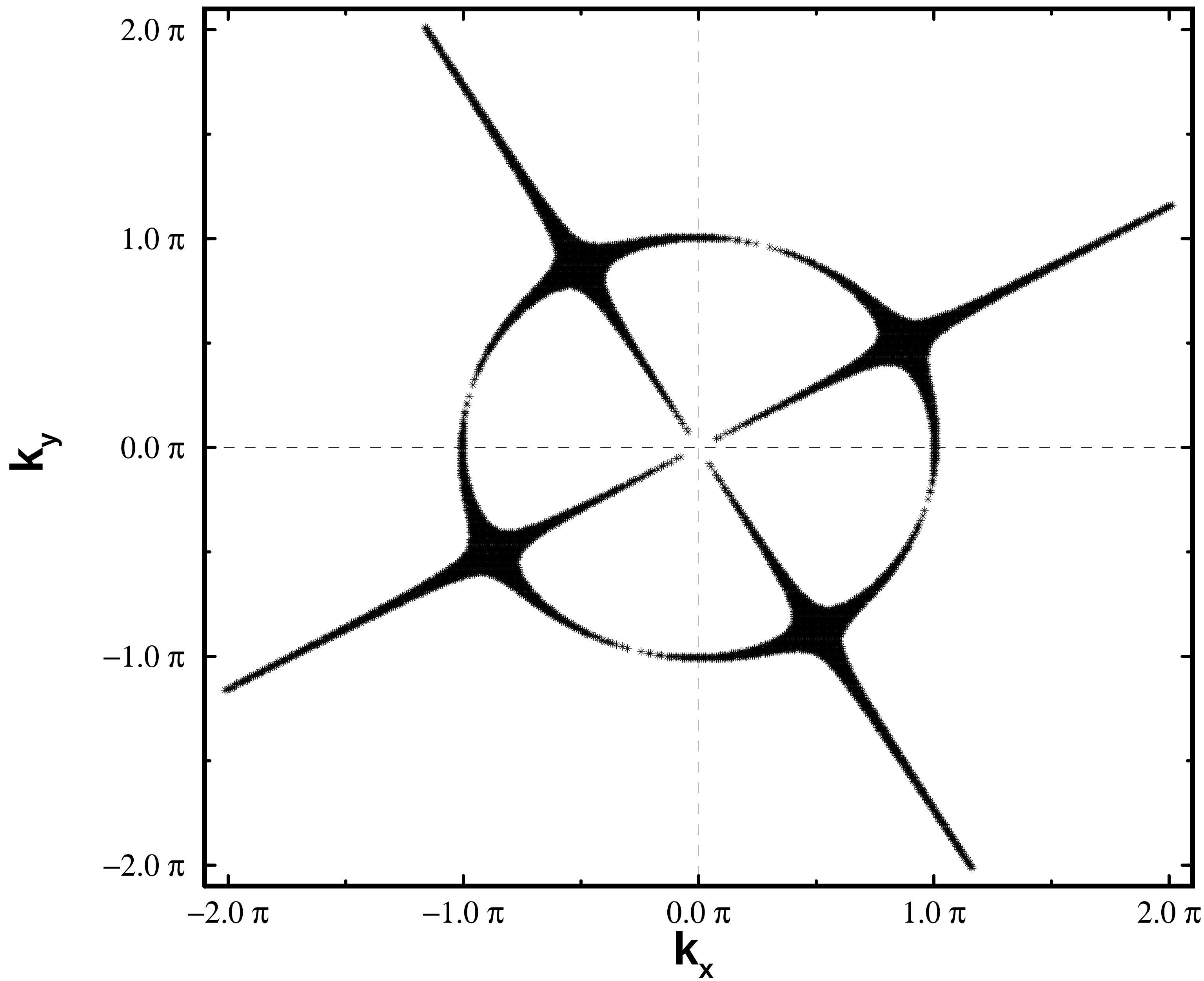

Fig. 4